

1-Nitropropane  
108-03-2 | DTXSID1020980

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

## Model Results

**Predicted value:** 6.47

**Global applicability domain:** Inside

**Local applicability domain index:** 5.84e-01

**Confidence level:** 8.77e-01

## Nearest Neighbors from the Training Set

Image not found

2-Nitropropane

**Measured:** 8.32

**Predicted:** 7.41

Image not found

Furan

**Measured:** 5.01

**Predicted:** 4.88

Image not found

2-Butanone oxime

**Measured:** 5.01

**Predicted:** 5.34

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Diethyl ether

**Measured:** 5.37

**Predicted:** 4.72

Image not found

Thiophene

**Measured:** 8.91

**Predicted:** 6.68